

## Behavior of different models of graphene under tension. Quantum chemical and finite element method calculations

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There are a number of physical models of graphene proposed in the various scientific disciplines that provide calculation of the mechanical properties. They correspond to different mathematical models, which, of course, often lead to discordant results. In this work the Young's modulus and Poisson's ratio for graphene sheet models have been calculated in the framework of the finite element method as well as using semi-empirical PM6 and DFT approaches.

We considered regular graphene sheets of different sizes and started from 3x3 cell. The next graphene sheet was obtained by increasing that cell on one hexagonal cell horizontally and on two cells vertically.

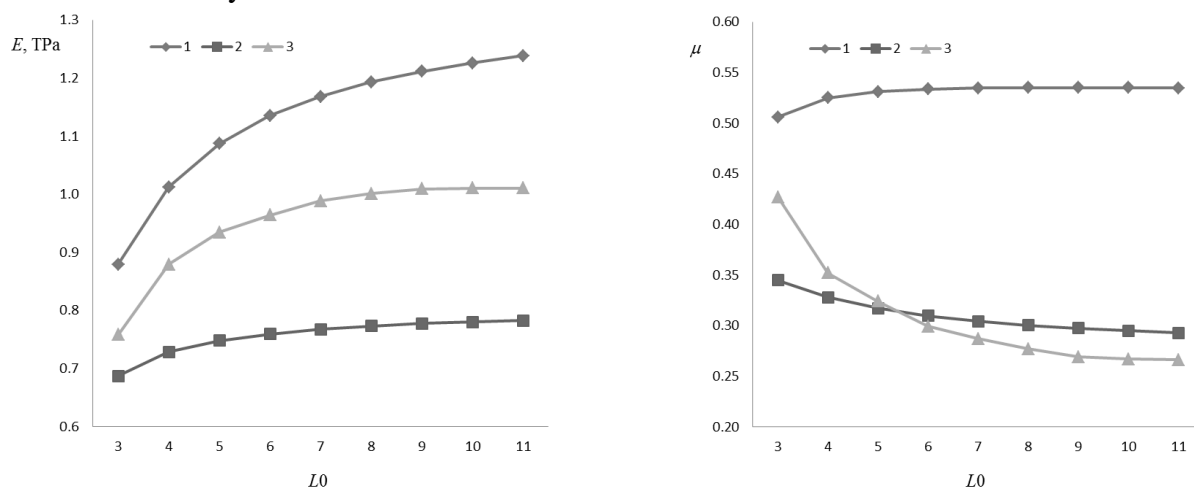


Fig. The calculated values of Young's modulus ( $E$ ) and Poisson's ratio ( $\mu$ ) depending of the number of cells ( $L_0$ ) along the horizontal axis:  
1 – central force field (CFF), 2 – valence force field (VFF), 3 – PM6

All three methods of calculations predict a monotonic increase in the Young's modulus with the rise of sample size with turning curves to asymptote for a bulk samples (Figure). Young's modulus value, calculated using quantum-chemical method PM6, lies between the values obtained using CFF and VFF methods. The results of DFT calculations of small graphene sheets are in a good agreement with those obtained using PM6 method.

The curves showing the dependence of the Poisson ratio of the size of the sample, calculated by different methods, differ significantly (Figure). The Poisson ratio, calculated using a CFF approximation, increases slightly with the rise of a sample size. However VFF and PM6 calculations predict a monotonic decrease of the Poisson ratio with the sample size increasing. Apparently, results of calculations using VFF approximation are not correct.

Thus, the usage of the approaches of classical and quantum mechanics allows to increase the reliability of the results and adjust their input parameters. For example, it becomes possible to use general harmonic force field approximation in the finite element method, which will improve the results.